

Cooper problem in a lattice

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Cooper problem for interacting fermions is solved in a lattice. It is found that the binding energy of the Cooper problem can behave qualitatively differently from the gap parameter of the BCS theory and that pairs of non-zero center of mass momentum are favored in systems with unequal Fermi energies.

I. INTRODUCTION

Cooper found [1] out that in the presence of the quiescent Fermi sea attractively interacting electrons can form a bound state even if their total energy is larger than zero. In the absence of Fermi sea such bound state does not exist in a three-dimensional system in a continuum although such a bound state may appear in quasi two-dimensional systems [2]. The possibility a bound state indicates instability and is traditionally thought of as an indicator of the instability towards the formation of a superfluid. However, the proper theoretical description of the superfluid itself involves a more refined many-body theory than the one used in the Cooper problem. The purpose of this report is to solve this classic Cooper problem in a lattice for a polarized system.

After formulating the Cooper problem in a lattice several questions are addressed. First, how does the binding energy behave and is it always qualitatively similar to the gap parameter in the BCS theory [3]? Second, what happens to the bound state in systems with unequal Fermi surfaces? Third, can bound states of non-zero center of mass be favorable in systems with unequal Fermi surfaces? This question is of interest since in the BCS theory one expects modulated, FFLO-type [4, 5], order parameters in systems with mismatched Fermi surfaces. Since optical lattices for ultracold atoms can be made anisotropic and spin-dependent, the problem is framed and solved in a rather general setting with spin-dependent lattice potentials.

Previously some aspects of the two-body problem in a lattice have been investigated in the absence of Fermi seas in Refs. [6, 7, 8]. Dimensionality effects in the Cooper problem were discussed by Esebbag *al.* [9].

II. FORMALISM

We assume a two-component system and we label the spin states by $\sigma = \{\uparrow, \downarrow\}$. If the system is composed of ultracold neutral fermionic atoms, these "spin" states would correspond to either different atoms or different

hyperfine levels of the same isotope. We further assume that atoms are at zero temperature and in a cubic lattice which is deep enough so that only the lowest band must be considered. Also, since the lattice is deep it is enough to consider only the leading order nearest neighbor tunneling processes with tunneling strengths \mathbf{t}_σ where bold-face indicates that the tunneling strengths are represented as vectors and that the tunneling strength can be different in different directions.

At zero temperature fermions on different spin states can interact via *s*-wave interaction and we take the interaction between unequal fermions located at lattice sites \mathbf{x}_\downarrow and \mathbf{x}_\uparrow to be $g\delta(\mathbf{x}_\downarrow - \mathbf{x}_\uparrow)$. Two-body wavefunction for the atoms is then a solution of the Schrödinger equation

$$\left[-\sum_{\sigma} \mathbf{t}_{\sigma} \cdot \nabla_{\sigma}^2 + g\delta(\mathbf{x}_{\downarrow} - \mathbf{x}_{\uparrow}) \right] \psi(\mathbf{x}_{\downarrow}, \mathbf{x}_{\uparrow}) = E\psi(\mathbf{x}_{\downarrow}, \mathbf{x}_{\uparrow}).$$

Here $\mathbf{t} \cdot \nabla^2$ denotes the discrete kinetic energy operator and it acts as

$$-\mathbf{t} \cdot \nabla^2 \psi(\mathbf{x}) = -\sum_{\alpha} t_{\alpha} [\psi(\mathbf{x}_{\alpha} + d) - 2\psi(\mathbf{x}_{\alpha}) + \psi(\mathbf{x}_{\alpha} - d)],$$

where $d = 1$ is the lattice constant and $\alpha \in \{x, y, z\}$. Since the interaction only depends on the relative coordinate it is useful to write the problem in terms of the wave-function for the relative coordinate $\mathbf{x} = \mathbf{x}_{\downarrow} - \mathbf{x}_{\uparrow}$. The center of mass and relative motion no longer separate in a lattice, but interactions do not couple different center of mass states to each other. We write the wave-function as

$$\psi(\mathbf{x}_{\downarrow}, \mathbf{x}_{\uparrow}) = \Pi_{\alpha \in \{x, y, z\}} e^{iK_{\alpha}(c_{\alpha}x_{\downarrow, \alpha} + (1-c_{\alpha})x_{\uparrow, \alpha})} \psi(\mathbf{r}), \quad (1)$$

where \mathbf{c} is yet to be determined coefficient related with the center of mass coordinate in a lattice. Since the center of mass and the relative coordinate do not separate, the algebra is somewhat more complicated than in a continuum, but nevertheless straightforward. It turns out that the coefficients c_{α} are determined by the equation

$$\frac{t_{\downarrow, \alpha}}{t_{\uparrow, \alpha}} = \frac{\sin(K_{\alpha}(1-c_{\alpha}))}{\sin(K_{\alpha}c_{\alpha})}. \quad (2)$$

If the lattice is spin independent the left hand side is equal to one and $c_{\alpha} = 1/2$. This corresponds to the usual center of mass transformation for equal mass atoms. If \uparrow -component is very heavy, the left hand side becomes very

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large and the coefficient $c_\alpha \rightarrow 0$, which again conforms to our intuition about the center of mass coordinate. However, in case of general spin dependent lattice potentials, coefficients must be solved using Eq. (2).

The Schrödinger equation for the relative coordinate then becomes

$$\left[\sum_{\alpha} \mathbf{E}(\mathbf{K})_{\alpha} \nabla_{\alpha}^2 + 2(t_{\downarrow, \alpha} + t_{\uparrow, \alpha} + \mathbf{E}(\mathbf{K})_{\alpha}) + g\delta(\mathbf{x}) \right] \psi(\mathbf{x}) = E\psi(\mathbf{x}), \quad (3)$$

where

$$\mathbf{E}(\mathbf{K})_{\alpha} = -t_{\downarrow, \alpha} \cos(K_{\alpha} c_{\alpha}) - t_{\uparrow, \alpha} \cos(K_{\alpha}(1 - c_{\alpha})).$$

By expanding the relative coordinate wave function

$$\psi(\mathbf{x}) = \frac{1}{Nd^3} \sum_{\mathbf{q}} \psi_{\mathbf{q}} e^{i\mathbf{q} \cdot \mathbf{x}}, \quad (4)$$

where N is the number of lattice sites, we find

$$\begin{aligned} & \frac{1}{N} \sum_{\mathbf{q}} \sum_{\alpha} \{ [2\mathbf{E}(\mathbf{K})_{\alpha} (\cos(\mathbf{q}_{\alpha}) - 1) \\ & + 2(t_{\downarrow, \alpha} + t_{\uparrow, \alpha} + \mathbf{E}(\mathbf{K})_{\alpha})] - E \} \psi_{\mathbf{q}} e^{i\mathbf{q} \cdot \mathbf{x}} \\ & = \frac{-g}{N} \sum_{\mathbf{q}} \psi_{\mathbf{q}} e^{i\mathbf{q} \cdot \mathbf{x}} \delta(\mathbf{x}). \end{aligned} \quad (5)$$

By multiplying with $e^{-i\mathbf{k} \cdot \mathbf{r}}$, summing over lattice sites, and defining $\alpha = \sum_{\mathbf{q}} \psi_{\mathbf{q}}$, we find an equation

$$\frac{-1}{g} = \frac{1}{N} \sum_{\mathbf{q}} \frac{1}{f(\mathbf{K}, \mathbf{q}) - E}, \quad (6)$$

where

$$\begin{aligned} f(\mathbf{K}, \mathbf{q}) &= \sum_{\alpha} 2\mathbf{E}(\mathbf{K})_{\alpha} (\cos(\mathbf{q}_{\alpha}) - 1) \\ &+ 2(t_{\downarrow, \alpha} + t_{\uparrow, \alpha} + \mathbf{E}(\mathbf{K})_{\alpha}). \end{aligned}$$

The crucial ingredient of the Cooper problem is the presence of the occupied Fermi seas. Due to Pauli blocking the two-body wavefunction cannot have amplitudes for those states that are already occupied. This restricts the sum-over the first Brillouin zone $\sum_{\mathbf{q}}$ into just a sum over allowed states $\sum'_{\mathbf{q}}$. If the Fermi energies are $\epsilon_{F, \sigma}$ and the free dispersions are $\epsilon(\mathbf{q})_{\sigma} = \sum_{\alpha} 2t_{\sigma, \alpha}(1 - \cos(\mathbf{q}_{\alpha}))$, then in practice this means that one should only include those modes \mathbf{q} that satisfy $\epsilon(\mathbf{q} + \mathbf{cK})_{\downarrow} > \epsilon_{F, \downarrow}$ and $\epsilon(-\mathbf{q} + (\mathbf{1} - \mathbf{c})\mathbf{K})_{\uparrow} > \epsilon_{F, \uparrow}$ simultaneously.

By using Eq. (6) one can solve for the pair energy E and investigate whether solutions with energies less than $\epsilon_{F, \downarrow} + \epsilon_{F, \uparrow}$ exist. For this reason it is helpful to write $E = \epsilon_{F, \downarrow} + \epsilon_{F, \uparrow} - \Delta$ so that $\Delta > 0$ for bound states. Due to the anisotropy and generally complicated structure of the Fermi surfaces, integrations are performed numerically.

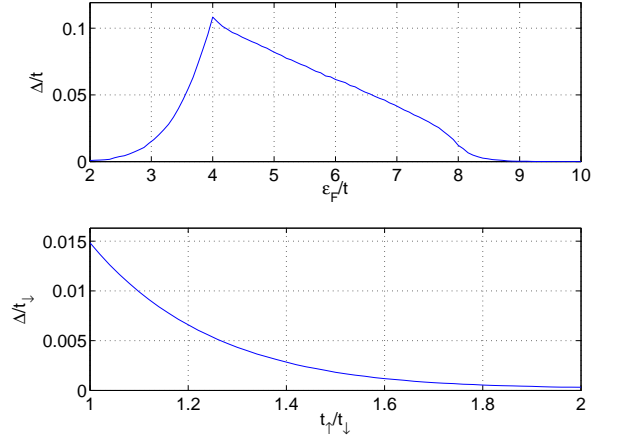


FIG. 1: Binding energy in a symmetric lattice with $g = -3t_x$ as a function of Fermi energy (top) and effective mass ratio (bottom) with $\mu_{\sigma} = 3t_{\sigma}$.

III. BINDING ENERGY IN SYMMETRIC LATTICES

Fig. 1 shows the binding energy as a function of Fermi energy for a system where both components see an equal and symmetric lattice as well as a system where the effective masses of the fermions are different. In the first case, the binding energy first rises quickly with the Fermi energy, but at $\epsilon_F = 4t$ the topology of the Fermi surface changes from closed to open. For higher values of the Fermi energy the binding energy decreases monotonically. Due to the particle-hole symmetry the gap parameter of the BCS theory is symmetric with respect to $\epsilon_F = 6t$ (which corresponds to half-filling and maximum gap parameter in the BCS theory). Such symmetry is absent in the Cooper problem. The behavior at small Fermi energies, which correspond to low filling fractions, is similar to the usual free space Cooper problem. Fig. 1 also shows the binding energy for the case when fermions have different effective masses i.e. when $t_{\uparrow} \neq t_{\downarrow}$. As the \uparrow -component becomes heavier the binding energy is reduced. This behavior is qualitatively similar to the behavior of the BCS gap parameter and is to a good accuracy exponential in the mass ratio.

In free space the solution to the Cooper problem predicts a binding energy $\Delta \sim \exp(-2/\lambda)$ while the BCS theory predicts a gap parameter $\Delta_{BCS} \sim \exp(-1/\lambda)$, where $\lambda = n(\epsilon_F)|g|$ and $n(\epsilon_F)$ is the density of states at the Fermi-energy. Therefore, for a similar coupling strength the binding energy in the Cooper problem is $\Delta \sim \Delta_{BCS}^2$, which is much smaller than Δ_{BCS} in the weak coupling regime. In a lattice, Δ is also much smaller than Δ_{BCS} , but generally the relation between these two quantities is more complicated. As the Fig. 1 demonstrates, the binding energy of the Cooper problem, is more sensitive to the structure of the Fermi-surfaces than the BCS gap parameter.

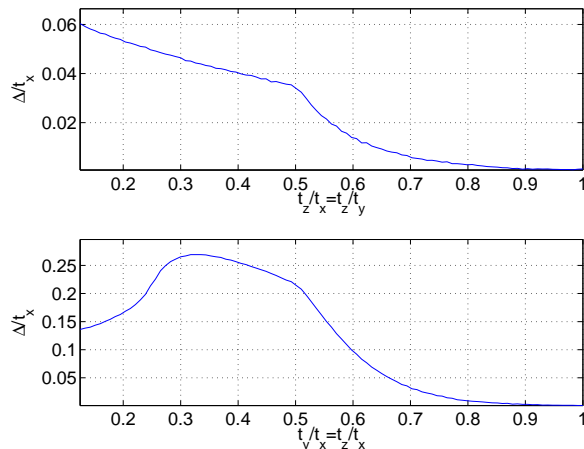


FIG. 2: Binding energy as a function of tunneling strength anisotropy for transitions into quasi-2D (top) and quasi-1D (bottom) situations. We choose $\epsilon_{F,\downarrow} = \epsilon_{F,\uparrow} = 2t_x$ and $g = -3t_x$.

IV. BINDING ENERGY AND DIMENSIONAL CROSSOVERS

If one makes the lattice anisotropic, one can effectively change the dimensionality of the system. In Fig. 2 demonstrates the effect of such changes in two cases. On the top part one changes the tunneling strength along z -direction while keeping other tunneling strengths the same. For small values of t_z the lattice is deep in the z -direction and the system is effectively a set of quasi-two-dimensional systems. As t_z/t_x increases to $\mu/4$ the structure of the Fermi surfaces change from open (cylinder shaped) Fermi-surfaces into a closed (cigar shaped) ones. This change is reflected as a kink in the binding energy of the Cooper problem.

The bottom part of Fig. 2 shows the binding energy for a system where t_y and t_z are varied, but kept equal to one another. For small values of t_y and t_z the system is effectively one-dimensional and Fermi surfaces are disconnected. Then the Fermi surface is composed of two sheets with no intersecting points. At $t_y = t_z = \mu/8$, the Fermi surfaces become connected, but are still open. The surfaces become connected so that the corners of the previously disconnected sheets merge first. As the tunneling strengths in y - and z -directions increase further, at $t_y = t_z = \mu/4$, the Fermi surfaces become closed and resemble the Fermi surfaces in a continuum in that sense. These changes in the Fermi surface topology are again reflected as kinks in the binding energy. Also in this case the binding energy is qualitatively different from the BCS gap parameter, which decreases monotonically as $t_y/t_x = t_z/t_x$ increases. In the one-dimensional limit fluctuations are important and the simple BCS mean-field theory is unreliable. It is interesting that the two-body Cooper problem avoids some qualitative problems faced by the BCS theory.

V. BOUND STATES OF NON-ZERO CENTER OF MASS MOMENTUM

In a two-component fermionic gas the atom numbers of different components can be independently controlled and such strongly interacting polarized fermion gases have been recently studied experimentally [10, 11, 12]. in a harmonic trap. Studies of polarized fermionic gases have revealed the possibility of phase separation [13] as well as the possibility of FFLO type order parameters which break the translational symmetry [14]. Due to nesting these modulated order parameters are expected to be more prominent in lattices [15] and in systems with reduced dimensionality [16, 17].

In the BCS theory at $T = 0$ the non-zero order parameter can exist for Fermi energy differences of order $\delta\epsilon_F = \epsilon_{F,\uparrow} - \epsilon_{F,\downarrow} \sim \sqrt{2}\Delta_{BCS}(\delta\epsilon_F = 0)$ [18]. We have verified that a similar conclusion applies for the existence of the bound state in the Cooper problem in the lattice. I.e. the bound state exists if $\delta\epsilon_F$ is (roughly) less than the binding energy Δ at $\delta\epsilon_F = 0$.

In an unpolarized system chemical potentials are the same and the Fermi surfaces are also the same. Then the binding energy of the Cooper problem is maximized at zero center of mass momentum due to the reduced density of available low energy states for non-zero pair momentum. However, when the system is polarized the Fermi surfaces are different and this argument is not necessarily valid anymore. Then non-zero pair momentum might be favorable just like FFLO-type states can appear in the BCS theory.

As Fig. 3 demonstrates, for systems with unequal Fermi surfaces the binding energy can indeed be maximized at non-zero center of mass momentum. If the Fermi energy difference is too large the bound state does not exist, but for Fermi energy differences which are less than about $\Delta(\delta\epsilon_F = 0)$ the possibility of non-zero center of mass pair must be taken into account. Fig. 3 also shows the binding energy in a quasi one-dimensional lattice. The binding energy of the non-zero center of mass pair is typically much larger in the one-dimensional system than a three-dimensional one. In the figure the binding energies in three-dimensional and one-dimensional systems are roughly similar in magnitude only because the average Fermi energy was lower in the quasi one-dimensional problem. One-dimensional system is qualitatively different from the three-dimensional one in that as Fermi energy difference increases the existence of bound states persists to larger center of mass momenta. This is reminiscent of the BCS theory in one-dimensional systems where there is no upper critical polarization above which the order parameter disappears.

VI. CONCLUSIONS

In summary, we solved the Cooper problem in a lattice and found that the behavior of the binding energy of the

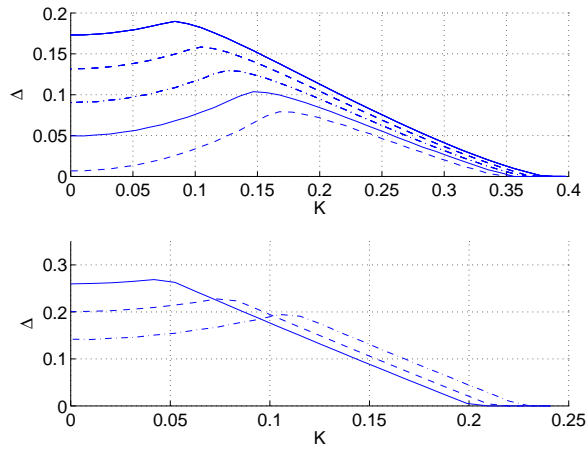


FIG. 3: Binding energy as a function of pair center of mass momentum (along x -direction) for few different Fermi energy differences $\delta\epsilon_F$. Top figure: the three-dimensional lattice was symmetric, $\bar{\epsilon}_F = (\epsilon_{F,\uparrow} + \epsilon_{F,\downarrow})/2 = 4t_x$, $g = -4t_x$, and (from top to bottom) $\delta\epsilon_F/\bar{\epsilon}_F = \{0.04, 0.05, 0.06, 0.07, 0.08\}$. Bottom figure: lattice was quasi one-dimensional with $t_y = t_z = t_x/10$, $\bar{\epsilon}_F = 3t_x$, $g = -4t_x$, and (from top to bottom) $\delta\epsilon_F/\bar{\epsilon}_F = \{0.03, 0.05, 0.07\}$.

Cooper problem is qualitatively different from the behavior of the gap parameter of the BCS theory. Also, for systems with different Fermi energies, if the instability exists it is towards the formation of pairs with non-zero center of mass momentum. In three dimensions at zero temperature the BCS theory for a polarized system predicts FFLO ordering only above certain non-zero Fermi energy difference [14, 15]. For smaller Fermi energy differences phase separation is expected to occur [13]. In contrast, the Cooper problem with mismatched Fermi surfaces always predicts instability towards non-zero center of mass pairs.

Two new interesting articles [19, 20] discussing the two-body scattering in an one-dimensional lattice in the absence of Fermi seas have appeared after the submission of this report.

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